Interactions and Interferences of Cu, Cr and As During Contaminated Waste Wood Gasification: A Thermodynamic Equilibrium Study

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***Abstract*—Waste wood (WW) is one of the major sources of renewable energy. However, it often contaminated with metal(loid) elements at concentrations leading to toxicity emissions and damages to facilities during thermal conversion. Thence, procedures for preventing and/or reducing the negative impacts of these elements require further understanding, specifically their phase transformations during thermal conversion processes. Although it is well known that phase transformation depends on different factors such as vaporization characteristics of elements, operational conditions and process configuration, influences of atmosphere composition of the reaction are rarely investigated. Based on thermodynamic equilibrium principles, this study investigates the behaviors of most regulated elements (Cu, Cr and As) in contaminated WW in relation to the presence/absence of Ca, Na, S, Cl, Fe and Ni during gasification. Thermodynamic calculations were performed across gasification temperature range of 0-1800°C, under the atmospheric pressure. Refinement of possible interactions and interferences reveals that Ni-As interactions generate dominant species As_2Ni_5 and As_8Ni_{11}, which increase the solid-gaseous transformation temperature of As. Furthermore, interactions between Ca and Cr predominantly forms C_3Cr_7; whereas absence of Ca leads to form $Cr_2Na_2O_4$ which causes instability in Cr phase formation. The findings of this study indicate that the evaluation of speciation due to interactions and interferences can provide quantitative and qualitative assessments of the metal(loid) behavior in gasification.**

***Keywords*—Waste Wood; Elemental Contaminants; Interactions; Interferences; Gasification; MTDATA.**

I. INTRODUCTION

The term waste wood (WW) refers to the wood that has previously been employed for different purposes, and can be used for energy production [1]. Waste wood comprises a wide variety of wood materials primarily resulted from demolition and construction operations, and from industrial and commercial activities [2][3]. Due to its diverse sources, WW is a highly homogeneous solid fuel containing both physical and chemical contaminants [1][4]. Physical contaminates can easily be separated by sorting or using mechanical methods. However, the major chemical contaminants usually linked to metal(loid) elements contained in wood that resulted from preservations, paintings, coatings, and other related activities, and of course, mechanical separation is inapplicable.

Currently, gasification is widely used as an advanced thermochemical conversion process due to its efficiency and flexibility [5]. It can simultaneously achieve considerable waste reduction and generate renewable energy. However, when conducting gasification, metal(loid)s in WW can cause severe human health and environmental problems as well as significant technical damages when they exceed acceptance concentration levels. Procedures for avoiding and/or limiting the risks of metal(loid)s require further understanding, particularly their behaviours during gasification.

A range of studies [6]–[10] in relation to the fate of metal(loid) elements in gasification process have focused on the distribution of these elements across gaseous and solid phases. These studies report that the partitioning of metal(loid) elements can be directly affected by a combination of several factors including feedstock characteristics, operation conditions, and process agents. Indeed, phase transformation temperatures of such elements cannot be precisely determined using conventional analysis due to the formed species cannot be easily identified and measured. Accordingly, mass distribution of metal(loid)s in gasification process is a rather complex problem.

Nevertheless, thermodynamic equilibrium modelling based on Gibbs energy minimisation has successfully been exploited for obtaining a best prediction of the behaviour of metal(loid) elements as well as evaluating the speciation during thermochemical processes [11]–[18].

Jiang et al. [11] studied the phase transformations of Al, As, Cd, Co, Cr, Cu, Fe, Mn, Mg, Ni, Pb and Zn present in five biomass samples in typical gasification scenarios. This study showed the most volatilized elements are Cd, Pb, Zn and As, whilst Mn, Cu, Co and Ni moderately volatilized; the phase transition temperatures of Cr, Fe, Mg and Al> 1200 °C. Froment et al. [12] performed thermodynamic equilibrium calculations to assess the volatilization and condensation of some elements present in woody biomass during gasification at temperature range from 500 to 1500 °C, under pressure conditions from 1 to 10 bar. Simulation results demonstrated that Zn, Hg, Pb, Cd, Se, F, Cl, Sb, S and N completely volatilized as either elemental or species, whereas, Ca, P, Si, Al, Ti, Fe, Cu, Mn, Cr, Ba and Mg remained as oxides in the

condensed phase, except copper which condensed as Cu_3As. Kramb et al. [13] modelled the behavior of As during the gasification of CCA-treated wood, and showed that above 99.6% of As can be captured. Thompson and Argent [14] grouped the behavior of trace elements in Prenlfo gasifier into "virtually immobile (Cr, Ni, Ba, V), somewhat mobile (Mo, Cu, Be), mobile (Sb, B) and almost totally mobilized (As, Cd, Pb, Sn, Zn)". Kilgallon et al. [15] showed the partitioning of trace elements in gasification products, and investigated the impacts of both pressure conditions and chlorine/sulphur on elements phase transformations. Reed et al. [16] presented the speciation prediction of As, B, Be, Cd, Co, Cu, Pb, Sb, Sn, V and Zn in fuel gas from a gasifier. They categorized these elements into three groups: condensed phase (Be, Co, Cu, V, and Zn; at $T_{50} \gg 900K$), gas phase (As without Ni, B without Ca, Sb, and Sn), and condensed phase (As with Ni, B with Ca, Cd, Pb; at $T_{50} < 900K$). Liu et al. [17] also presented the speciation distribution of As, Cd, Ni, Pb, Sb and Se during underground coal gasification under specific agent injection and pressure. A study by Bradshaw et al. [18] showed that eight elements (As, Cd, Hg, Pb, Te, Sb, Se, and Sn) and alkali metals remained in fuel gas, and species of Cd, Pb and Sb could be passed through the path of fuel gas forming surface deposits.

Although most of the phase transformation models can provide useful information (e.g. operation conditions, vaporization, condensation) about metal(loid) elements partitioning, factors such as interactions and interferences between these elements cannot be disregarded. Particularly, metal(loid)s can be interacted or interfered each other's, generating new species which may lead to appreciable influence on the volatilization of metal(loid) elements. To date, to the best of authors' knowledge, there has been no single study attempts to assess the effect of occurred interferences between metal(loid)s during thermochemical processes. However, only a study by K. Svoboda [19] investigated the simultaneous interferences of both HCl and HF on H_2S sorption. In addition, only two studies evaluated the impact of interactions on element behaviour during coal combustion. Contreras et al. [20] assessed the interactions between the trace elements As, Hg, Cd, and Sb, and reported that some species can be dominant under certain conditions. For instance, As-Cd interaction forms $Cd_3(AsO_4)_2$ specie, which may reduce gaseous oxides concentration. Yan et al. [21] showed the interactions between As, Hg, and Se can lead to form AsSe(g) and HgSe(g) which considered dominant species under reducing conditions.

The primary objective of this paper is to explore the possible interactions and interferences between the most regulated metal(loid)s in contaminated WW, thereafter investigate the impact of generated species on their distributions in gasification process. Contaminated WW samples with complete composition data were selected from the ECN PHYLLIS2 database [22]. Thermodynamic equilibrium calculations were performed using MTDATA software (Version 5.10, NPL, UK) to model the phase transformations of CCA elements during the gasification followed by speciation assessments.

II. THERMODYNAMIC EQUILIBRIUM MODELLING

Thermodynamic equilibrium modelling of gasification was carried out using multiphase module of MTDATA software (Ver. 5.10 NPL, UK) coupled with Scientific Group Thermodata Europe (SGTE) database to predict both phase transformation and speciation formation of Cu, Cr and As in WW. A primary search of SGTE database was conducted to reveal the relevant speciation of these elements. A complete list of the selected species for modelling is given in Table I.

TABLE I. LIST OF CCA-ELEMENT SPECIES INCLUDED IN THE MODELLING.

Metal(loid)	Solid species	Liquid species	Gaseous species
Cu	$AsCu_3$,$AsCu_3O_4$,$As_2Cu_3O_8$,CCuN,$CCuO_3$,CaCu,$CaCu_5$,Ca_2Cu,$CaCu_2O_3$,Ca_2CuO_3,ClCu,Cl_2Cu,Cu,$CuFeO_2$,$CuFe_2O_4$,$Cu_2Fe_2O_4$,$CuFeS_2$,Cu_5FeS_4,CuH_2O_2,CuH_2O_5S,CuH_6O_7S,$CuH_{10}O_9S$,CuO,Cu_2O,CuO_4S,Cu_2O_4S,Cu_2O_5S,CuS,Cu_2S		ClCu,Cl_2Cu,Cl_2Cu_2,Cl_3Cu_3,Cl_4Cu_2,Cl_4Cu_4,Cl_5Cu_5,Cu,Cu_2,CuH,CuHO,CuO,CuS,Cu_2S
Cr	$AsCrO_4$,$As_2Cr_3O_8$,C_2Cr_3,C_3Cr_7,C_6Cr_{23},C_6CrO_6,$CaCrO_3$,$CaCr_2O_4$,Cl_2Cr,Cl_3Cr,$CoCr_2O_4$,Cr,Cr_2FeO_4,CrN,Cr_2N,$CrNa_2O_4$,$Cr_2Na_2O_4$,Cr_2NiO_4,CrO_2,CrO_3,Cr_2O_3,Cr_5O_{12}, Cr_8O_{21},$Cr_2O_{12}S_3$, CrS.		ClCr,Cl_2Cr,Cl_3Cr,Cl_4Cr,Cl_5Cr,Cl_6Cr,ClCrO,$ClCrO_2$,Cl_2CrO,Cl_2CrO_2,Cl_3CrO,Cl_4CrO,Cr,Cr_2,CrH,CrHO,$CrHO_2CrHO_3$,CrH_2O_2,CrH_2O_3,CrS_2,CrH_2O_4,CrH_3O_3,CrH_3O_4,CrH_4O_4,CrH_4O_5,CrN,CrO,CrO_2,CrO_3,Cr_2O,Cr_2O_2,Cr_2O_3,CrS.
As	As,$As_2Ca_3O_8$,,$As_2Co_3O_8$,$AsCrO_4$,$As_2Cr_3O_8$,AsS,$AsNa_3$,$AsCu_3$,$AsCu_3O_4$,$As_2Cu_3O_8$,$As_2Fe_3O_8$,$AsFeO_4$,$AsNa_3O_4$,AsNi,As_2Ni_5,As_8Ni_{11}, As_2S_2,$As_2Ni_3O_8$, As_2O_5, As_2S_3.	As_4S_4, $AsCL_3$	As,As_2,As_3,As_4,$AsCl_3$,AsH,AsH_2,AsH_3,AsN,AsO,AsO_2,As_4O_6,As_4O_7,As_4O_8,As_4O_9,As_4O_{10},AsS,As_4S_4

The best fit probability distributions of composition data of the selected WW samples (#2712, #1779, #1448, #1364, #871, #679, #3498, #2900, #2901) [22] are estimated using @Risk analysis simulation package (Ver.6.1, Palisade Corp. Ithaca, NY, USA), and given in Table II. To systematically explore possible interactions and interferences, the mass range of each minor element (Table III) assumed based on the information provided by PHYLLIS2 database [22] regarding the contaminated woody biomass. The elements to be introduced to MTDATA comprise major elements (C, H, N, Ar, and O) and minor elements (As, Cu, Cr, Ca, Cl, Co, Fe, Ni, Na, and S).

The operational conditions and process agents are presented in Table IV. In this table, the required oxygen for gasification determined using the following equation [23].

$$C + 0.5O \rightarrow CO \quad (1)$$

The Air composition under standard dry at atmospheric pressure consists of 75.47% N_2, 23.2% O_2, 1.28 % Ar, and

0.046% CO_2. Biomass feed rate is calculated based on higher heating value (2) for contaminated WW [23].

$$HHV_d = 0.3491C + 1.1783H + 0.1005S - 0.015N - 0.1034O - 0.0211Ash \quad (2)$$

TABLE II. ESTIMATED COMPOSITION DATA.

Component	Basis	Weight	Component	Dry Weight (mg/Kg)
Moisture	Ar	14.86%	Cu	63.64
Ash	Ar	12.09%	Ni	15.69
C	Dry	46.555%	As	5.5
H	Dry	5.69%	Co	4.88
N	Dry	1.06%	Cr	30.2
O	Dry	40.65%	Na	703.92
S	Dry	0.090%	Ca	4061.41
Cl	Dry	556.49mg/Kg	Fe	655.96

TABLE III. ASSUMED MASS FLOW OF MINOR ELEMENTS.

Element	Concentration (mole/h)	Element	Concentration (mole/h)
As	0,0.7,1.4,5	Fe	0,50,100,500
Cu	0,4,6,8	Ni	0,5,10,20
Cr	0,5,10,21	Na	0,100,200,500
Ca	0,100,250,500,1000	S	0,0.05,0.1,0.2
Cl	0,l0,50,100		

TABLE IV. SIMULATION PARAMETERS FOR GASIFICATION.

Parameters	Range/Value
Temperature range (°C)	0-1800
Pressure (atm)	1
Equivalence ratio	0.2
Biomass rate (Kg/h)	3.59
Air rate (m^3/h)	0.72
Steam rate (m^3/h)	1.44
Steam /Air	2:1

III. RESULTS AND DISCUSSION

A. Partioning behaviours of CCA-element (Cu, Cr and As)

The calculation procedure commenced with considering composition data and process parameters in Table II and Table IV, respectively. The predicted equilibrium partitioning of CCA elements depicted in Fig. 1, 2 and 3.

The obtained results show that, at temperatures ≤ 1350°C, about 100% of Cu remained in solid phase as dominant specie CaCu which is formed by Ca-Cu interaction, Fig. 1. As the temperature increases from 1350 to 1800°C, new gaseous species CuCl (5.5E-3-55.44E-2%), CuH (0.47-4.49%), and Cu_2 (0.02-0.43%) are formed due to Cl-Cu and H-Cu interactions. At temperature ranged from 1450 to 1600°C, Cu proportionally partitioned into elemental between solid phase (88.84-33.57%) and gaseous phase (4.29-94.52%).

Chromium predicated as solid specie C_3Cr_7 at temperatures up to 1550°C, originated from C-Cr interaction. Further, at temperature ranged of 1550-1800°C, the mass percentage of C_3Cr_7 decreased from about 100 to 67.34%. At the same temperature range, it is released as elemental Cr (3.16-32.48%) and a new set of gaseous species is generated from Cl-Cr, H-Cr, N-Cr and O-Cr interactions, Fig. 2. However, the total mass percentage of these species is less than 0.2%.

With regard to As distribution, Fig. 3, the results show that As remained in solid phase at temperatures ≤ 1400°C. This is mainly due to the generation of the stable species $AsNa_3$ (100%) and As_2Ni_5 (99.99-99.15%) from Na-As interaction and Ni-As interaction, respectively. At temperatures above 1400°C, the mass percentage of As decreases rapidly in solid phase, and regenerates as a new gaseous species mostly by interactions. Among these species, the dominant ones are As (5-46.55%), As_2 (1.90-46.00%) and AsH (0.24-7.13%). Indeed, AsH generated from H-As interaction.

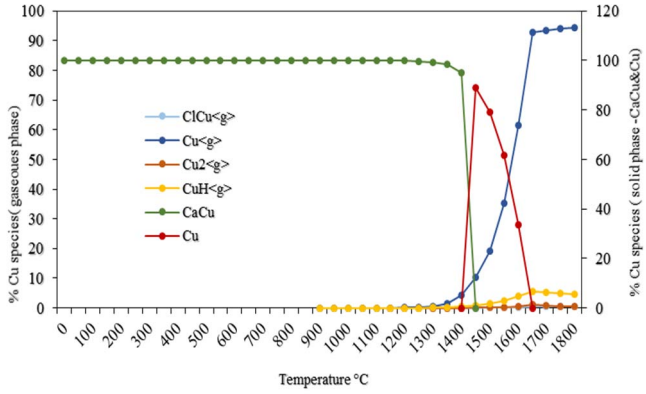


Fig. 1. Speciation of Copper.

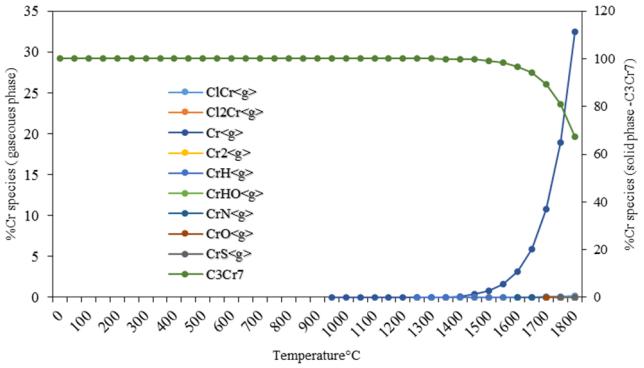


Fig. 2. Speciation of Chromium.

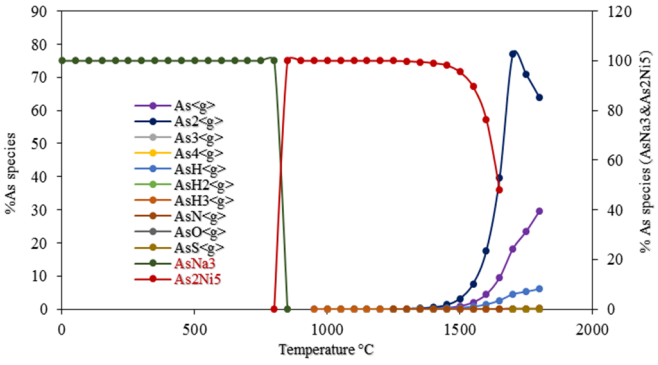


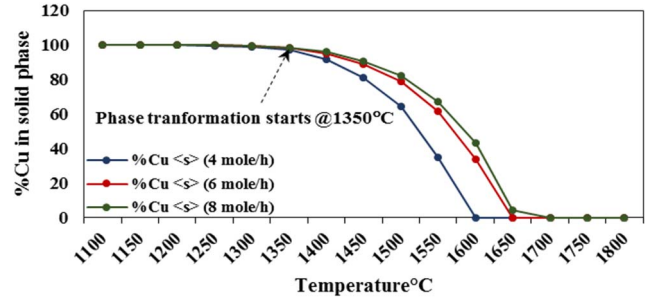
Fig. 3. Speciation of Arsenic.

B. Influence of elements contents

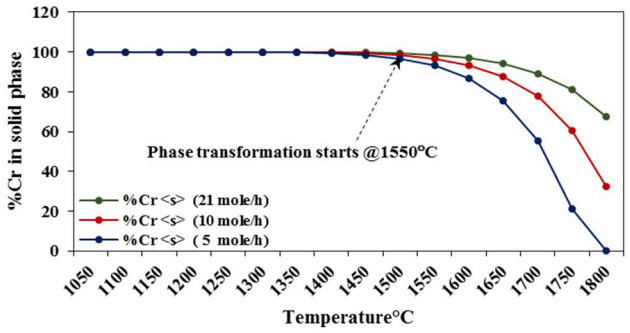
The calculation directed to predict possible interactions and interferences that may occur when elements contents are varied according to concentrations assumed in Table III. It is important to note here that, occurred interactions/interferences that cause appreciable influences on both phase and speciation formation ranked as significant interactions/interferences.

1) Effect of CCA

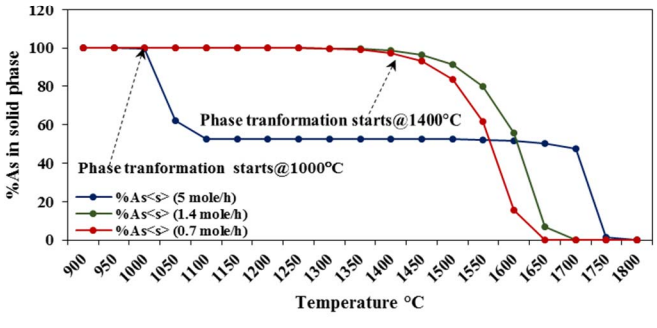
In this case, the concentration of Cu, Cr and As are individually changed. The results indicate that CCA-element contents in the model have almost no effect on their phase transformation temperatures and only concentration shifts are observed as shown in Fig. 4(a, b, and c). However, an exception is that when As concentration is relatively high (5 mol/h), its phase transition temperature decreased by 400°C due to Ni contained becomes lower than the limit to interact with As and hence capture 100% of As. In addition, As_2Ni_5 (solid-phase) and AsN (gaseous-phase) are the dominant As species.



a) Cu solid transition.



b) Cr solid transition.



c) As solid transition.

Fig. 4. Phase transformations of CCA elements when different concentrations are considered.

2) Effect of Ca, Na, S, Cl, Fe, and Ni on CCA elements partitioning

A summary of the occurred interactions and interferences between CCA-element and individual presence/absence of each of Ca, Na, S, Cl, Fe and Ni are depicted in Fig. 5. Further details are given in following parts.

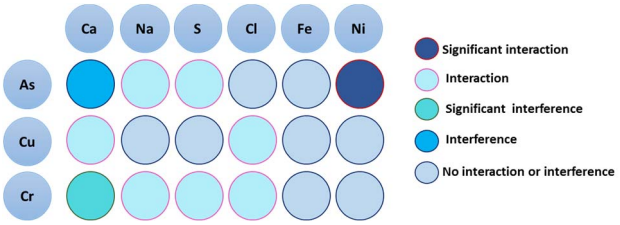


Fig. 5. The occurred interactions and interferences.

a) Arsenic

When Ni is present at different levels, all Ni-As interactions form solid specie As_2Ni_5, thereby the phase transformation temperature of As (Fig. 6) increases to about 450°C. In contrast, the absence of Ni implies generation of As_2 (gaseous) and $AsNa_3$ (solid) as the dominant species (Fig. 7). Similarly, Na-As interacts to form $AsNa_3$; however, the absence of Na shows no effects on the As phase formation, but enhances Ni to capture As generating As_2Ni_5 (100-99.15%) up to 1400°C (Fig. 8). The presence of S tends to form, at very low mass percentage, gaseous specie AsS between 1750 and 1800°C.

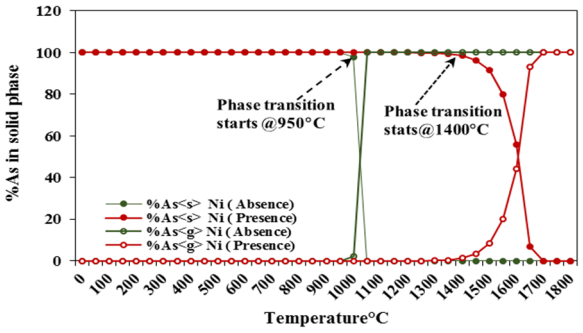


Fig. 6. Arsenic partitioning when Ni presence/absence.

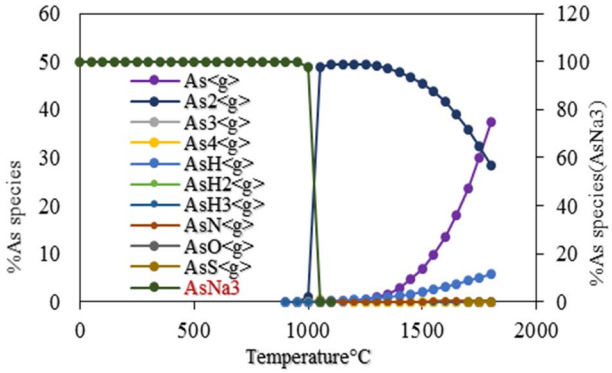


Fig. 7. Arsenic speciation formation in absence of Ni.

As a result of Ca-As interference, AsS specie releases at 1750°C instead of 1200°C at which AsS released without Ca. This shift in temperature is caused by CaS specie that results from Ca-S interaction. This observation is consistent with the finding that the presence of Ca in the system can decrease As-S interaction [20].

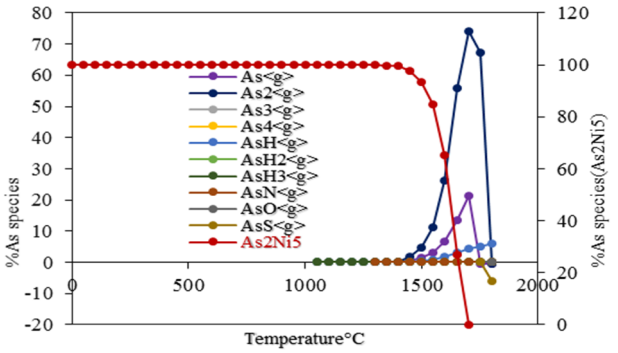


Fig. 8. Arsenic speciation formation in absence of Na.

b) Copper

The resulting species from the occurred Ca-Cu interactions are illustrated in Table V. The dominant species in solid phase are CaCu, CaCu & $CaCu_5$ and CaCu when Ca is present at levels of 250, 500, and 1000 mole/h, respectively. However, the presence of Ca at low concentration would not be enough to interact with Cu; instead, it interacts with both O and Cr, generating $CaCr_2O_4$ and CaO. It is notable that the volatilization of Cu is unaffected by the different levels of Ca. Similarly, Cl-Cu interactions only form gaseous specie CuCl between 1400 and 1800°C.

TABLE V. CALUCIUM-COPPER INTERACTIONS.

Concentration Ca (mole/h)	Species	Temperature range
100	Cu<s>	0-800
	Cu<s>,Cu<g>,CuH<g>	850- 950
	Cu<s>, ClCu<g>,Cu<g>,CuH<g>	1000-1800
250	CaCu<s>	0-800
	Cu<g>, CuH<g>,CaCu<s>	850-1150
	ClCu<g>,Cu<g>,Cu_2<g>, CuH<g> ,CaCu<s>	1350-1800
500	CaCu<s>,$CaCu_5$<s>	0-800
	Cu ,Cu<g>,CuH<g>	850- 950
	Cu<g>,CuH<g>,CaCu<s>	1000-1150
	ClCu<g>,Cu<g>,Cu2<g>, CuH<g> ,CaCu<s>	1250-1800
1000	CaCu<s>	0-800
	Cu<g>,CuH<g>,CaCu<s>	850- 950
	Cu<g>,CuH<g>,CaCu<s>	1000-1150
	ClCu<g>,Cu<g>,Cu_2<g>, CuH<g>, CaCu<s>	1250-1800

c) Chromium

Evaluation of possible interactions and interferences reveals that Ca has an important effect on Cr partitioning (Table VI and Fig. 9). In this sense, Na and Cr interacts only if the concentration of Ca ≤ 100 mole/h, forming instable solid specie $Cr_2Na_2O_4$ between 1100 and 1550°C. Also, $CaCr_2O_4$ (solid) is the most likely to be formed by Ca-Cr interaction when Ca is present at 100 mole/h, thereby about 100% of Cr remain in solid phase at temperatures ≤ 1550°C. As the calcium content increases (>100 mole/h), Ca-Cr interferences and C-Cr interactions occur simultaneously, generating C_2Cr_3 and C_3Cr_7 in solid phase at temperatures up to 1550°C. A most apparent observation in this case is the concentration shift in gaseous phase of Cr.

Other interactions, specifically, S-Cr and Cl-Cr interactions have no effect on Cr volatilization, and only form the gaseous species CrS and $ClCr\&Cl_2Cr$, respectively.

TABLE VI . CHROMIUM-CALCIUM INTERACTIONS.

Concentration Ca (mole/h)	Species	Temperature range
0	$Cr_2Na_2O_4$ <s>	0-300
	C_2Cr_3<s>,$Cr_2Na_2O_4$<s>	350-400
	$Cr_2Na_2O_4$<s>	450-600
	Cr<g>,C_2Cr_3,$Cr_2Na_2O_4$<s>	650-1200
	ClCr<g>,Cl_2Cr<g>,Cr<g>, CrHO<g>,CrS<g>,C_2Cr_3<s>, Cr<s>,C_3Cr_7<s>,C_6Cr_{23}<s>	1250-1800
100	C_2Cr_3<s>,$CaCr_2O_4$<s>, CrN<s>,$Cr_2Na_2O_4$<s>	0-300
	C_2Cr_3<s>,$Cr_2Na_2O_4$<s>	350-400
	C_2Cr_3<s>,$CaCr_2O_4$<s>	450-600
	ClCr<g>, Cr<g>, C_2Cr_3<s>,$CaCr_2O_4$<s>	650-1200
	ClCr<g>,Cl_2Cr<g>,Cr<g>, C_2Cr_3<s>	1250-1800
250- 500	C_2Cr_3<s>	0-300
	C_2Cr_3<s>,C_3Cr_7<s>	350-600
	C_3Cr_7<s>	650-1200
	C_2Cr_3<s>,ClCr<g>,Cl_2Cr<g>,Cr< g>,CrH<g>,C_3Cr_7<s>, CrO<g>,CrS<g>,CrN<g>	1250-1800
1000	C_3Cr_7<s>	0-600
	Cr<g>,C_3Cr_7<s>	650-1200
	ClCr<g>,Cl_2Cr<g>,Cr<g>, CrH<g>,CrO<g>,CrS<g>, CrN<g>, C_3Cr_7<s>	1250-1800

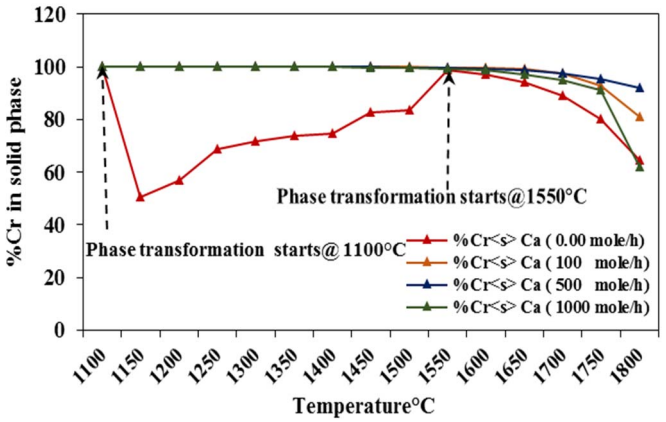
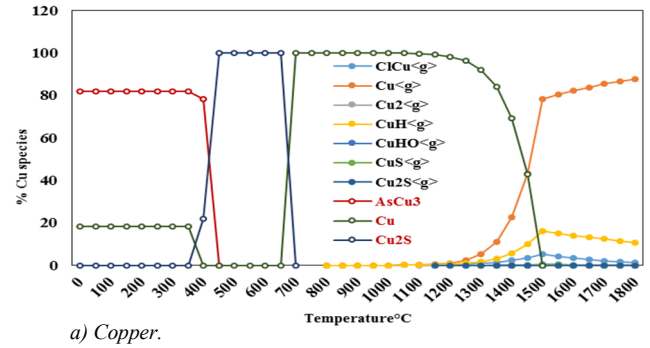


Fig. 9. Effects of Ca on Cr phase formation.

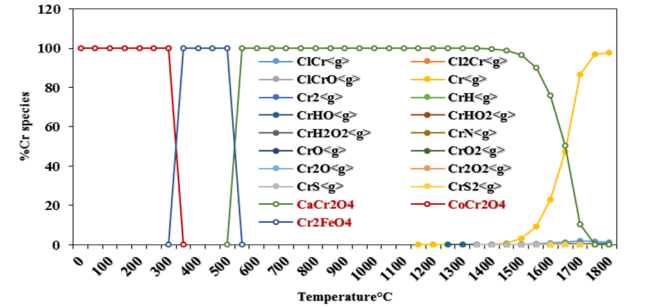
3) Effect of minor elements on CCA elements Partioning

All the minor elements are introduced to the model at the same concentration to identify significant interactions which ascribe to elemental reactivity, particularly CCA elements. The

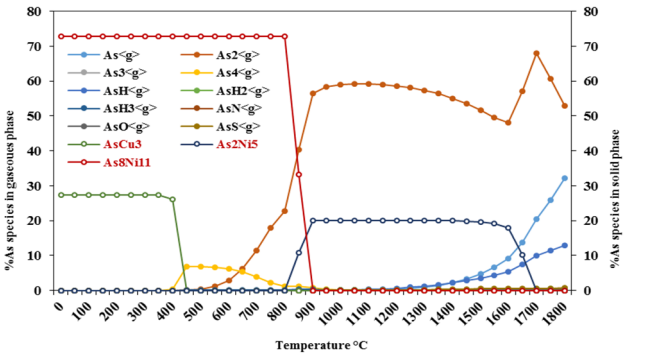
speciation formation of these elements are exhibited in Fig. 10 (a, b, and c).



a) Copper.



b) Chromium.



c) Arsenic.

Fig. 10. Speciation of CCA-element, when considering same concentrations of minor elements.

Results of Cu distribution between 0 and 700°C indicate that Cu interacts favorably with As and S to generate solid species $AsCu_3$ (81.89-78.24%) and Cu_2S (100%), respectively. At temperatures above 700°C, Cu is redistributed as elemental and set of gaseous species; however, the phase transformation temperature of Cu becomes 1200°C which is less than about 11% of that estimated in equilibrium composition (Fig. 1).

The predictive calculations originate Cr solid species $CoCr_2O_4$ (100% between 0-300°C), Cr_2FeO_4 (100% between 350-500°C) and $CaCr_2O_4$ (100% between 550-1450°C) to the Co-O-Cr, Fe-O-Cr and Ca-O-Cr interactions, respectively.

Fig. 10c shows As species formation. $AsCu_3$ (27.27% between 0-400°C) and As_8Ni_{11} (72.73% between 0-800°C) are the most probably solid species from Cu-As and Ni-As interactions, respectively.

In this view, the distribution profiles of CCA elements present significant trends towards their emissions control. More specifically, presence of Ni and S enhances As and Cu capture in ash, respectively. Copper and arsenic interactions cause both of them to remain in solid phase. Furthermore, the elements Ca, Co and Fe are favored to Cr retention.

IV. CONCLUSION

This paper provided a predictive model to understand the partitioning of CCA elements in terms of interactions and interferences during the gasification of contaminated WW. Refinement of obtained results shows that the occurrence of Ni-As interactions, and in most cases, leads to about 100% of As remaining in solid phase at temperatures up to 1400°C. Moreover, Ca-Cr interferences generate solid specie C_3Cr_7; however, absence of Ca causes instability in Cr behavior between 1100 and 1550°C. On the other hand, Co-O-Cr, Fe-O-Cr and Ca-O-Cr interactions decrease Cr volatilization as a result of the generation of solid species $CoCr_2O_4$, Cr_2FeO_4, and $CaCr_2O_4$, respectively. Finally, this modelling is valuable for mitigating the negative impacts associated with CCA elements, principally when systematically blending different types of contaminated WW. Consequently, better gasification and cost saving can be achieved.

V. REFERENCES

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